Status Report on the Wasatch Front Ozone Study

Principal Authors

Patrick Barickman
Robert Swart

Division of Air Quality
Department of Environmental Quality

150 N. 1950 West
Salt Lake City, UT 84116-3085

September 1997

TABLE OF CONTENTS

List of Figures

List of Tables

ACKNOWLEDGMENTS

1. INTRODUCTION

This report is the first in a series to document the conclusions of the first phase of the Wasatch Front Ozone Study (WFOS), begun in the Fall of 1994. The purpose of this document is to describe the background and context of the study, and to describe the analysis undertaken by the Utah Division of Air Quality (UDAQ) staff in deciding on a base case scenario to evaluate the ozone maintenance plan. The modeling protocol developed for this study and a report of the emissions preparations and quality assurance checks have been dealt with in detail by the contractor hired by UDAQ. Three areas which will be discussed in detail in this report are air quality/meteorology inputs to the model, diagnostic tests, and model performance evaluation. These are areas which the UDAQ staff has delved into at some length both to get a well grounded understanding of the model itself and to try to improve its performance by making the best use of the data at hand. Staff anticipates the completion of a second report, during the first quarter of CY98, containing more detailed diagnostic analyses of the model, model runs using projected year emissions inventories based on the ozone maintenance plan, and a time line and work program to develop a new episode based on a more complete data set from 1996.

This document should be viewed as a summary-type status report and not a complete WFOS project report. The brevity of this report should not be viewed as an indication of the extent of the overall project. Many sub-tasks, not reported here (nor in the contractor's final report), were necessary to arrive at this point. Some of these sub-tasks included the development of:

- temperature fields, based upon minimal data
- domain mean winds
- vertical atmospheric structure
- emissions, spatially, and temporally resolved
- accurate inputs for UAM-IV sub-program
- procedures for graphically viewing results with a geographic information system (GIS)

In addition to the extensive list of sub-tasks, the model itself was executed nearly 200 times; which also required numerous runs of the sub-program. Additionally, numerous meetings (in-house, with the Technical Review Panel, contractors and other interested parties) have been conducted since the project's inception in 1994.

2. BACKGROUND

A look at the yearly trend of ozone exceedence's over the last twelve years shows that generally NAAQS exceedences for ozone declined since the late 1980's. It is unclear whether this has been a result of regulatory policy, favorable meteorological conditions, or a combination of both. During the present decade the Wasatch Front has experienced a couple of summers with unusually cool and wet conditions. However, there have also been periods during the summer when meteorological conditions have been conducive to high ozone episodes, and the standard was not exceeded.

The conceptual model of the ozone problem along the Wasatch Front assumes that ozone builds up over a multi-day period with pollutants being trapped and recirculated in the urban air basin. The combination of high mountains to the east, and the Great Salt Lake to the west create down slope mountain/valley breezes which blow offshore to the Lake during the night and morning hours. This flow reverses during the afternoon and evening, creating on-shore and up-slope winds across the valley and up into the mountains.

Historical data shows a weekly trend of ozone concentrations building up during the work week with exceedences usually occurring during the latter part of the week, on a Thursday or Friday. Concentrations tend to fall off dramatically on the weekends and begin the pattern again at the start of a new work week. Although this pattern is not fully understood, it is thought that the urban area's pollutants are not necessarily being transported out of the region and dispersed into cleaner air. It is quite possible that during high ozone episodes the local wind patterns recirculate ozone and ozone precursors in the area which are subsequently added to a new batch of emissions day after day.

3. ANALYSIS UNCERTAINTIES

The primary difficulty in evaluating model performance is the fact that there exist only four ozone monitoring stations for the episode of July 21-22, 1988. In addition to the general lack of data to compare observed ozone concentrations with those estimated by the model, uncertainty also exists in characterizing conditions in the atmosphere, roughly between ground level and the tops of the mountain peaks. In addition, there are unknowns about background levels of pollution at the far edges of the model boundary as well as general uncertainty in emission factors such as those used to estimate volatile organic compounds (VOC) from automobiles.

File Contains Data for PostScript Printers Only

Figure 3.1. WFOS UAM-IV modeling domain

Common themes which often run through the reports of ozone studies from around the country are the lack of data to characterize the meteorology for a given episode and hour-specific emissions inventories. This study is no exception. Because of the varied and complex terrain of the area, which especially complicates wind flow, the lack of meteorological data adds a special burden. Figure 3.1 depicts the modeling domain and various meteorological monitoring sites (discussed below).
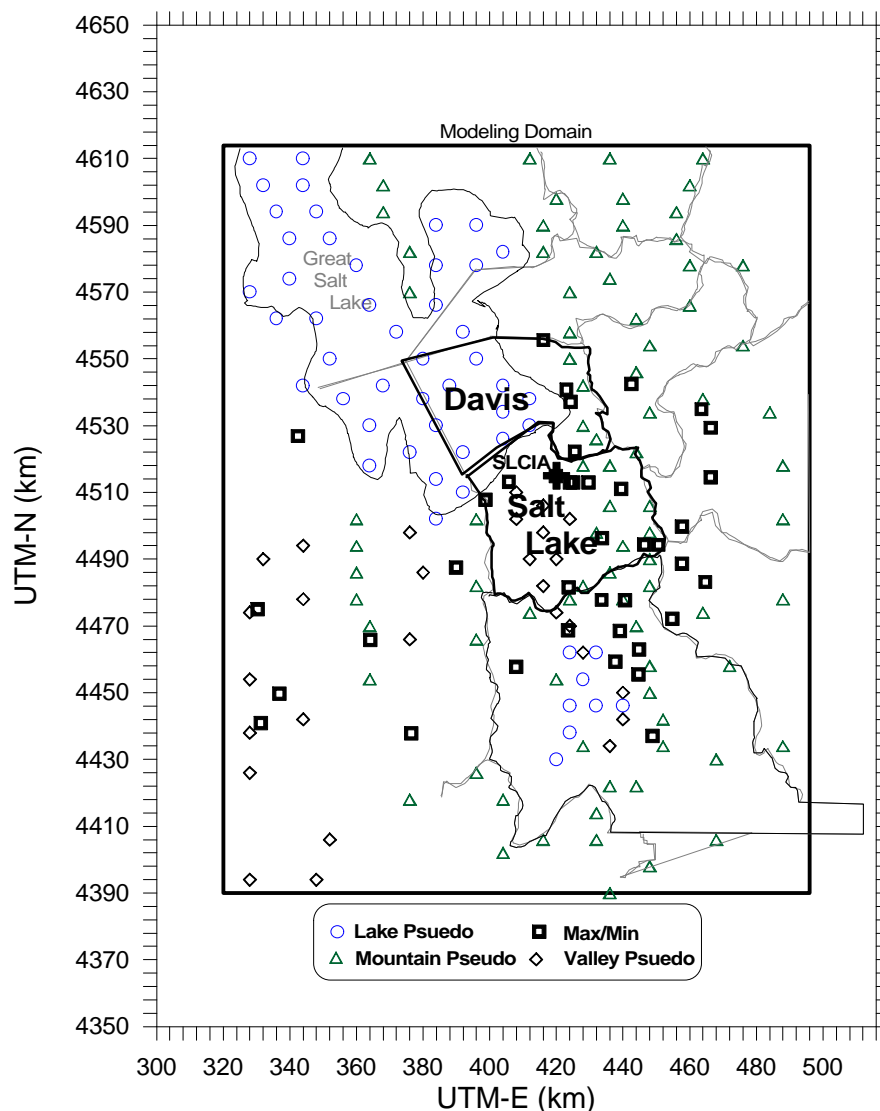
3.1 Meteorology

The contribution of upper air conditions in the pattern of wind recirculation and its contribution to ozone build up is thought to be significant. Unfortunately, the only upper air data available for this episode in 1988 comes from one monitoring station, with a launch frequency of twice-daily, at the Salt Lake City International Airport (SLCIA). There are a number of upper air parameters which must be estimated from this data. With only one upper air station the resultant vertical profiles of meteorological parameters cannot be adequately replicated, given the mountainous areas of the domain.

A significant amount of work was done in-house to create the best possible wind fields, given the data available. It has been determined that a sophisticated prognostic wind model, initially used by the outside UAM-IV contractor, was less accurate, with respect to end-results of ozone prediction, than the simpler, diagnostic wind model (DWM). Incorporated into the DWM model for this episode, is data from six meteorological stations at various locations around the Great Salt Lake. These stations were operational during the summer of 1996 for an intensive field study to collect more data for the UAM-IV model. Data from these stations were used as "pseudo data" in order to better characterize the influence of the lake on the wind fields. After perhaps fifty to one hundred different sensitivity runs with DWM, the wind fields are as well characterized as is possible, given the available data for this 1988 episode (see figure 3.1). As a general rule, it can be said that wind flows in mountainous terrain behave in very complex patterns, which are not represented well by observations on flat valley floors. A significant question remains as to whether the down slope air flow from the mountains was captured by the wind model.

Another area of the UAM-IV which received considerable attention from the UDAQ staff was in the characterization of the air temperatures near the ground surface, also known as the temperature field. This set of inputs influences the reaction rate of ozone chemistry in the lower levels of the atmosphere, and it is also a very important parameter in the calculation of the biogenic VOC emissions. The development of the surface temperature fields required a lot of attention for the same reasons as the wind fields. There was a general lack of data, with only one site at the SLCIA, gathering hourly averaged temperature data in 1988. In addition, with the large variation in terrain, i.e. the lake surface and the large change in elevation from the valley floor to the mountain peaks, more input data was needed to correctly characterize the temperatures across such a varied landscape.

Surface temperature fields were interpolated using the standard preprocessor within UAM-IV. However, inputs for the preprocessor were developed by searching out other sources of data to incorporate. This included approximately forty sites which had daily minimum and maximum temperature readings. Some of these stations were located in the mountains, others were located

in the valleys. These temperatures were interpolated in time by assigning the two observed values to maximum and minimum points on a cosine curve, and then interpolating temperature values for other hours along the curve. Other "pseudo stations" were needed to provide observation points for the UAM preprocessor's spatial interpolation method. Again, these pseudo stations were needed in order to characterize the different temperature regimes of the complex terrain. In order to get hourly temperature values for these pseudo sites, a change in temperature relative to elevation was estimated using a fixed lapse rate (change in temperature with height). The lapse rate was applied to the hourly temperatures at the airport to estimate pseudo temperatures in various parts of the domain. Finally, hourly Great Salt Lake water and air temperatures were correlated with hourly temperatures at the SLCIA. These correlated temperatures were then used to estimate hourly lake temperatures for those periods when "lake" data was unavailable. Figure 3.2 depicts the locations of the various "pseudo" temperature stations.

Figure 3.2. Pseudo temperature station locations

Two other significant meteorological parameters which were studied, but still require more detailed analysis are the three-dimensional temperature fields and mixing heights.

3.2 Emissions Inventory

The work done to create the emissions inventory for the model was fairly extensive from the outset. The UDAQ, in conjunction with the regional transportation planners (WFRC, MAG, UDOT, and the governor's Office of Planning and Budget), did a substantial amount of work to spatially disaggregate mobile and area source emissions to the proper grid cell location in the modeling domain. A GIS was used to grid mobile emissions and to convert 1990 census population into gridded population density. Population density was used as a surrogate to spatially distribute area source emissions as well as the portion of automobile emissions driven on local roads. The GIS was also used to create the most accurate and up to date land use and land cover data base possible for use in the biogenic emissions modeling. Temporal disaggregation was accomplished by applying time-of-day weighting factors, which were derived from EPA defaults or local data, if available. For example, on-road mobile emissions were weighted according to road use, taking into account rush-hour patterns.

A fairly detailed procedure was followed to assess and characterize the emissions inventories for the ozone episodes. This process is detailed in the contractor's final report (Reynolds, 1997). However, uncertainty remains in this component of the UAM-IV inputs. This is true for these types of modeling studies in many parts of the country. A study in Phoenix, Arizona pointed to two key areas of uncertainty in the emissions inventory during the evaluation of UAM-IV model performance. These are in the estimation of biogenic volatile organic compound (VOC) emissions and in oxides of nitrogen (NO_x) and VOC emissions from automobiles. Evaluation of model performance suggests that these two areas should also receive more study and analysis in future uses of the UAM-IV for the Wasatch Front.

4. MODEL PERFORMANCE EVALUATION

One of the uses of a functioning UAM is for evaluating the impact of emission control strategies. The evaluation of model performance is needed in order to determine the utility of the model for that purpose. The model evaluation is conducted after all sensitivity tests and refinements to model inputs have been made.

Model performance evaluations, both graphical and statistical, which are suggested by the Environmental Protection Agency's (EPA) guidance (EPA, 1994) are indicated below. Details of the model performance evaluation procedures are included in that document, as well as the modeling protocol (Tesche, 1994).

4.1 Graphical

Graphical displays can provide important information on qualitative relationships between predicted and observed concentrations. Listed below are the recommended (EPA, 1991) minimum displays:

- Time-series plots comparing hourly predicted and observed concentrations for each monitoring station (figure 4.1);

- Tile plots or tile maps of observed and predicted (lowest layer) concentrations for selected hours and for daily maxima (figures 4.3 - 4.5);

- Scatter plots of predictions and observations (figure 4.6) ; and

- Quantile plots (figure 4.7).

4.1.1 Time Series Plots

Figure 4.1 (a-d) depicts the comparison of observed vs. predicted ozone ("weighted 4" procedure) at the four monitors (Bountiful, Salt Lake, Cottonwood, and North Provo). Of significance are two key features evident in the comparisons:

1. All, with the exception of North Provo, show higher observed peak concentrations;

2. All predicted peaks occur a number of hours later than the observed peaks.

The later observation, i.e., predicted peak timing, may be an episode-specific artifact. The figure shows the average time of predicted ozone peaks at each station for the months of July and August, with respect to ozone with observed peaks greater than 100 ppb. The average time of peaks was 1:00 p.m., except for Cottonwood which was 2 p.m. Of particular interest, with respect to the observed peaks, is the deviation of Bountiful's monitor from the gradual buildup and decline of O_3 at a more typical monitor. The reason for this is not understood; regardless, this extreme peak will probably never be matched by UAM-IV simulations, due to limitations in both the model and the sophistication of model inputs.
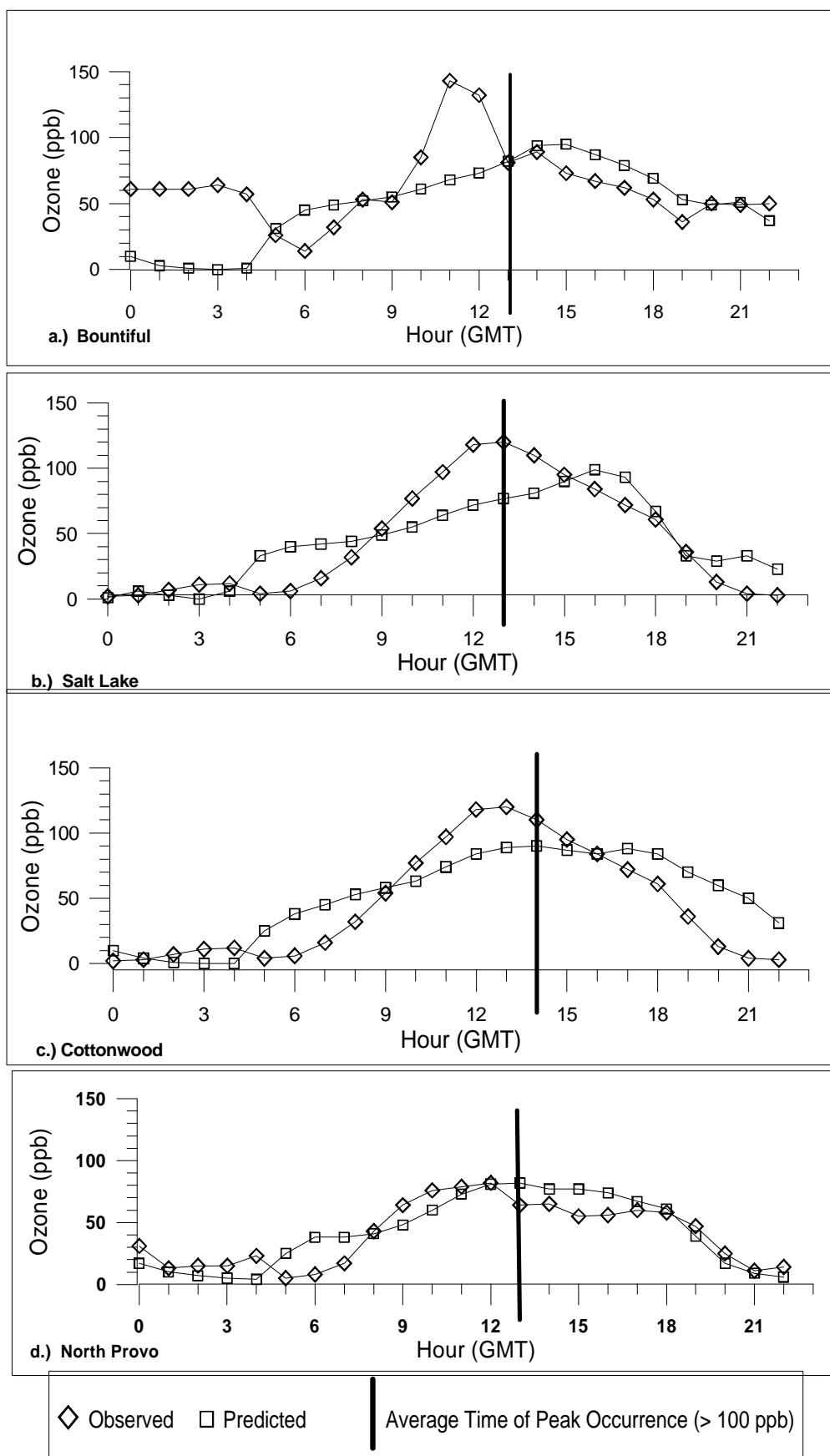
Figure 4.1. Comparison of monitored and predicted (w4) time series ozone for episode 2, July 21 - 22, 1988

4.1.2 Ground level tile plots.

A GIS is used for the visual analysis of ground level ozone concentrations. Instead of tile plots, gray shaded concentration surfaces are created which allows one to easily see the variation and movement of the ozone plume throughout the simulation. Figure 4.2 shows the model simulation at 11 a.m., Friday morning, July 22, 1988. The monitor at Bountiful recorded an hourly averaged ozone concentration of 143 parts per billion, the highest level of the day. As shown earlier, in figure 4.1a, this is a relatively steep spike of ozone which would be difficult for the model to capture, even if the simulation was producing higher levels of ozone during the morning hours.

File Contains Data for PostScript Printers Only

Figure 4.2. Ozone at the time of peak monitored ozone at Bountiful

Figure 4.3, shows the model simulation at 1 p.m. The monitor at Cottonwood reached its peak observed concentration at this time.

File Contains Data for PostScript Printers Only

Figure 4.3. Ozone at the time of peak monitored ozone at Cottonwood.

It is not until several hours later, at 4 p.m., that the model first generates an exceedence of the standard, and at 5 p.m. generates a peak estimated value of 131 parts per billion as shown in figure 4.4.

File Contains Data for PostScript Printers Only

Figure 4.4. Ozone at the time of peak predicted value.

The model attempts to simulate ozone development along the Wasatch Front in both time and space. The three figures above, 4.2, 4.3, and 4.4, illustrate the failure of the model, for this episode, to characterize the peak build up of ozone early enough in the day. The fact that the peak concentrations are not directly over the monitor locations and that the peak level of 131 ppb is slightly below the observed peak, is less troubling. With so few monitors to compare actual values to those estimated, and given the uncertainty in the emissions estimates, capturing the peak values in the general urbanized area indicates that the model is at least characterizing an ozone plume within the domain. Further work and analysis during the creation of a new episode for 1996 should be done in order to achieve a better temporal match, by estimating peak ozone earlier in the day.

4.1.3 Scatter Plots

Scatter plots depict the extent of bias and error in the ensemble of hourly prediction-observation pairs. Bias is indicated by the systematic positioning of data points above or below the perfect correlation line. The dispersion of points is a measure of the error in the simulation. The scatter plot also reveals outlier prediction-observation pairs.

Figure 4.5 shows a fair amount of over and under prediction, in relation to the perfect correlation line. The scatter does not appear to have any particular bias to either over or under predict. There are, however, some interesting biases that show up in the quantile plots, discussed below.
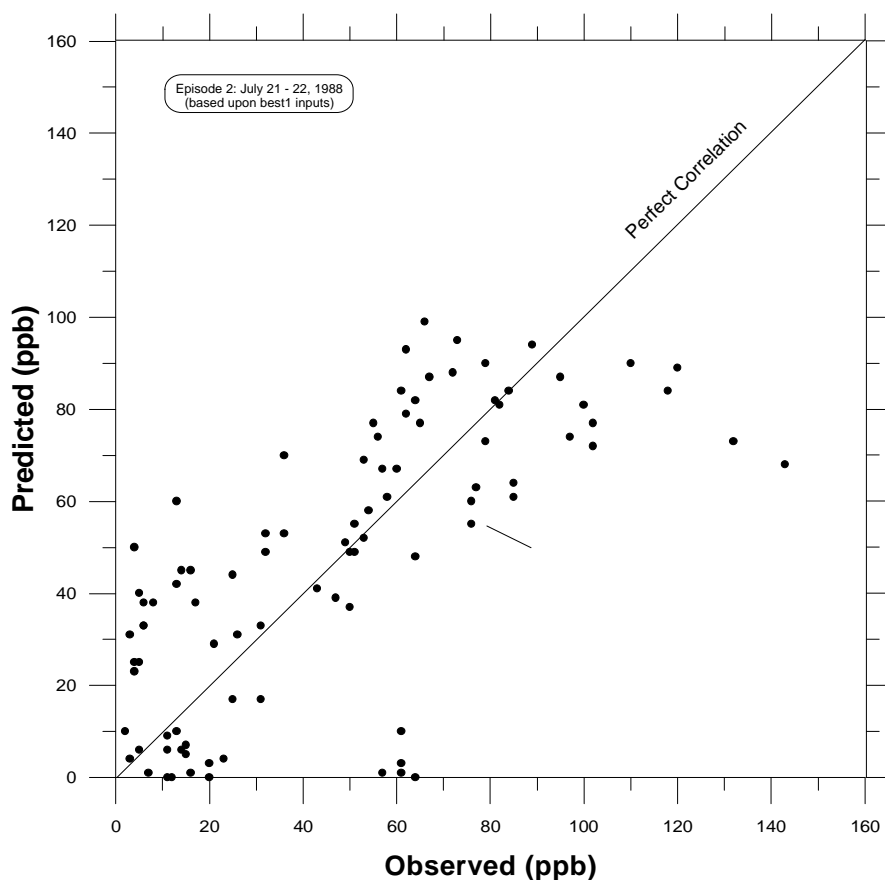
Figure 4.5. Scatter plot of all observed and predicted (wt4) ozone for episode 2, July 21 - 22, 1988)

4.1.4 Quantile-Quantile plots

Quantile-Quantile plots compare the frequency distributions of rank-ordered observed and rank-ordered predicted concentrations. The observed and predicted concentrations are sorted from highest to lowest, then plotted on an x-y plot. This graphically depicts any model bias over the frequency distribution.

The quantile-quantile plot comparing the observed and the "weighted 4" predicted ozone (figure 4.6) shows a degree of bias in two particular areas; namely, extreme low values (20 - 40 ppb, and extremely high values. In the distributions below 40 ppb, there is a bias of over prediction, and with values higher than approximately 100 ppb, there is an extreme under prediction. The time series plots corroborate this conclusion. The hour by hour points show an over prediction a few hours before and after the peak. As discussed previously, the actual peaks are significantly under predicted, thus confirming the bias depicted in the quantile plot.
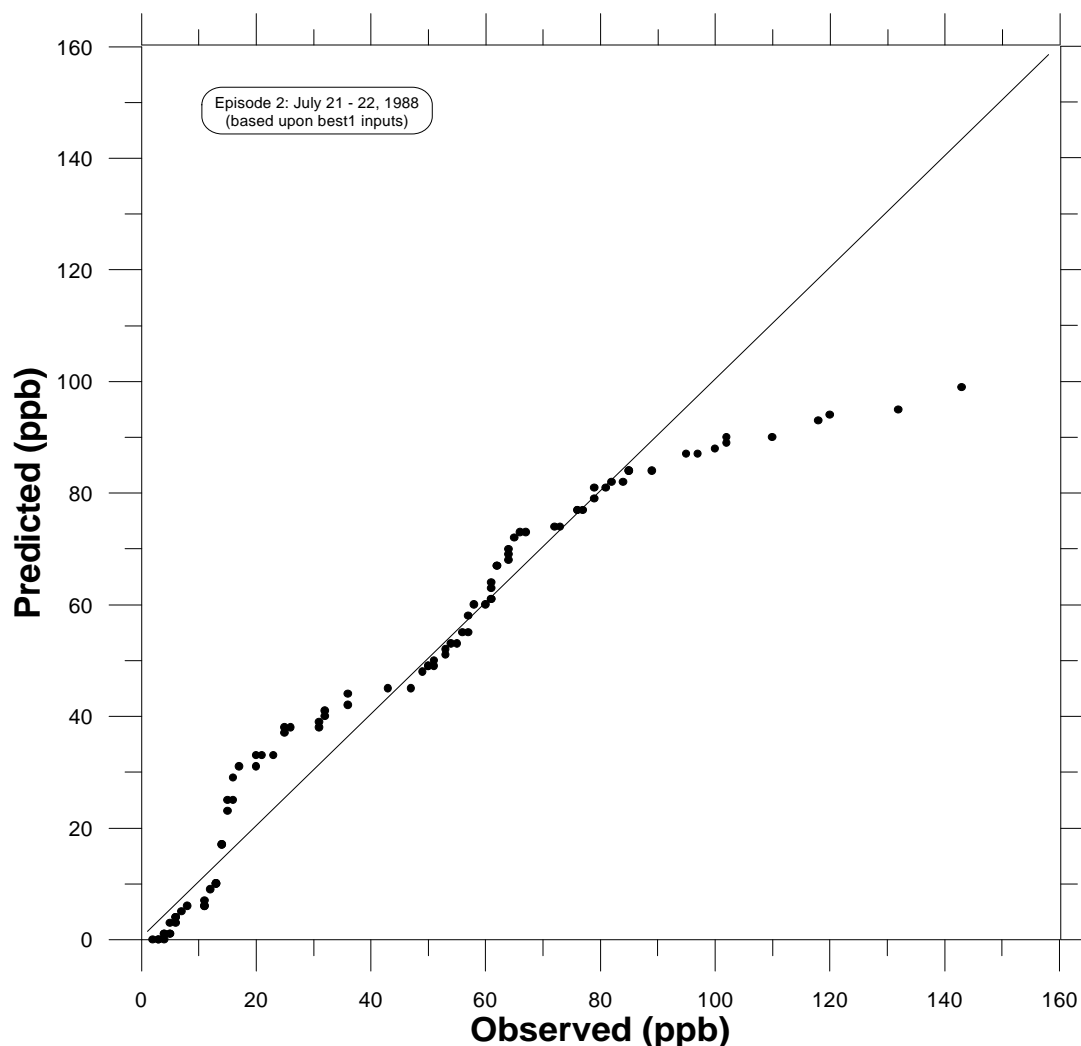
Figure 4.6. Quantile-Quantile plot of all observed and predicted (wt4) ozone for episode 2, July 21 - 22, 1988

4.2 Statistical

Statistical performance measures can provide meaningful measures of model accuracy for dense monitoring networks. However, statistical measures may give a distorted view of model performance in cases of routine monitoring networks, where coverage may be sparse. Although the recommended statistical measures should be applied, caution is suggested for interpreting these measures in cases of sparse monitoring network coverage. The WFOS monitoring network, four sites in the domain, is considered quite sparse and therefore strict pass/fail judgements cannot be made on the statistics alone. Consequently, the statistics discussed below must be viewed in light of a very sparse network, and conclusions drawn could be somewhat tenuous. EPA (1991, 1994) recommends the following statistical performance measures:

- Unpaired highest-prediction accuracy;

$$A_u = \frac{c_o(.,.) - c_p(.,.)}{c_o(.,.)} \times 100\%$$

- Normalized bias test of all pairs with observations above 60 parts per billion (ppb);

$$D^* = \frac{1}{N_T} \sum_{i=1}^{N} \sum_{j=1}^{Hi} \frac{c_o(i,j) - c_p(i,j)}{c_p(i,j)}$$

and

- Gross error of all pairs with observations above 60 ppb.

$$E_d^* = \frac{1}{N_T} \sum_{i=1}^{N} \sum_{j=1}^{Hi} \frac{|c_o(i,j) - c_p(i,j)|}{c_p(i,j)}$$

where

A_u = unpaired highest-prediction accuracy (quantifies the difference between the magnitude of the highest 1-hour observed value and the highest 1-hour predicted value)

E_d^* = normalized gross error for all hourly prediction-observation pairs for hourly observed values > 60 ppb

$c_o(.,.)$ = maximum 1-hour observed concentration over all hours and monitoring stations

$c_p(.,.)$ = maximum 1-hour predicted concentration over all hours and surface grid squares

D^* = normalized bias obtained from all hourly prediction-observation pairs

N = number of monitoring stations

H_i = number of hourly prediction-observation pairs for monitoring station I

N_T = total number of station hours

$$= \sum_{i=1}^{N} H_i$$

$c_o(i,j)$ = observed value at monitoring station I for hour j

$c_p(i,j)$ = predicted value at monitoring station I for hour j

Table 4-1 below, shows the results of the statistical tests and compares each with its respective, recommended value. Two different procedures were used in determining the "predicted" values. The first, "weighted 4," is the weighted average of the predictions from the four grid cells nearest to, and including, the monitoring station. The four-cell weighted average, the procedure recommended in the guidance (EPA, 1994) is derived from bilinear interpolation (Tesche, 1990). The second procedure , "best of 9," is the best "prediction" selected from the nine grid squares surrounding and including the monitor. As can be seen, each of the three tests, regardless of the "prediction" procedure, resulted in acceptable values.

Table 4-1. Statistical Performance of UAM

TEST	Acceptable Range (%)	Calculated Values (%)	
		Weighted 4	Best of 9
Unpaired Highest-Prediction Accuracy (A_u)	15-20	8	8
Normalized Bias > 60 ppb (D)	5-15	13	8
Gross Error of All Pairs > 60 ppb (E_d)	30-35	31	17

Based upon both the graphical and statistical reviews, it is assumed, by the UDAQ staff, that episode 2 (July 21-22, 1988) has been adequately developed for limited use in control strategy studies.

5. CONCLUSIONS

In general, the UDAQ staff views the work, completed to date, as being very instructive as to the ozone formation process and transport mechanisms. The work that has been reported here was conducted in parallel with a portion of the work that was initiated through a consortium of independent contractors. That work has been completed and UDAQ has received the final report. The executive summary of that report is reproduced as Appendix A to this document. There are a few differences in the conclusions drawn from that initial work and the efforts reported herein. UDAQ staff took the modeling effort beyond that of the contractors and made many improvements in modeling approaches and inputs; namely wind fields, temperature fields, and upper level atmospheric parameters.

Listed below are a number of initial conclusions that can be drawn from both the contractors' and staffs' efforts:

1. The WFOS airshed appears to be VOC limited. That is, with decreases in NO_x there is an associated increase in maximum ozone concentrations. Table 5-1 shows the maximum predicted ozone concentrations (ppb) with various levels of precursor reductions. Figure 5.1 is a plot of the relationship of the reductions included in table 5-1. Strategies to reduce VOC are the most effective in reducing the peak ozone concentrations simulated with UAM. Reducing NO_x, while holding VOC emissions steady, actually increases peak ozone concentrations. This has implications for policies which reduce nitrate emissions for PM_{fine} pollution in that controls to reduce nitrates could cause ozone concentrations in the urban areas to increase.

Table 5-1. VOC/NOx reduction effects upon O3 maximum concentration.

	NOx Reductions (%)						
VOC Reductions (%)	0	5	10	15	20	30	40
0	131	134	137	139	142	151	160
5	128	131	134	136			
10	124	128	131	133	135	141	152
15	121	124	128	131			
20	119	124		130			
30	116		117			128	
40	113		114				126
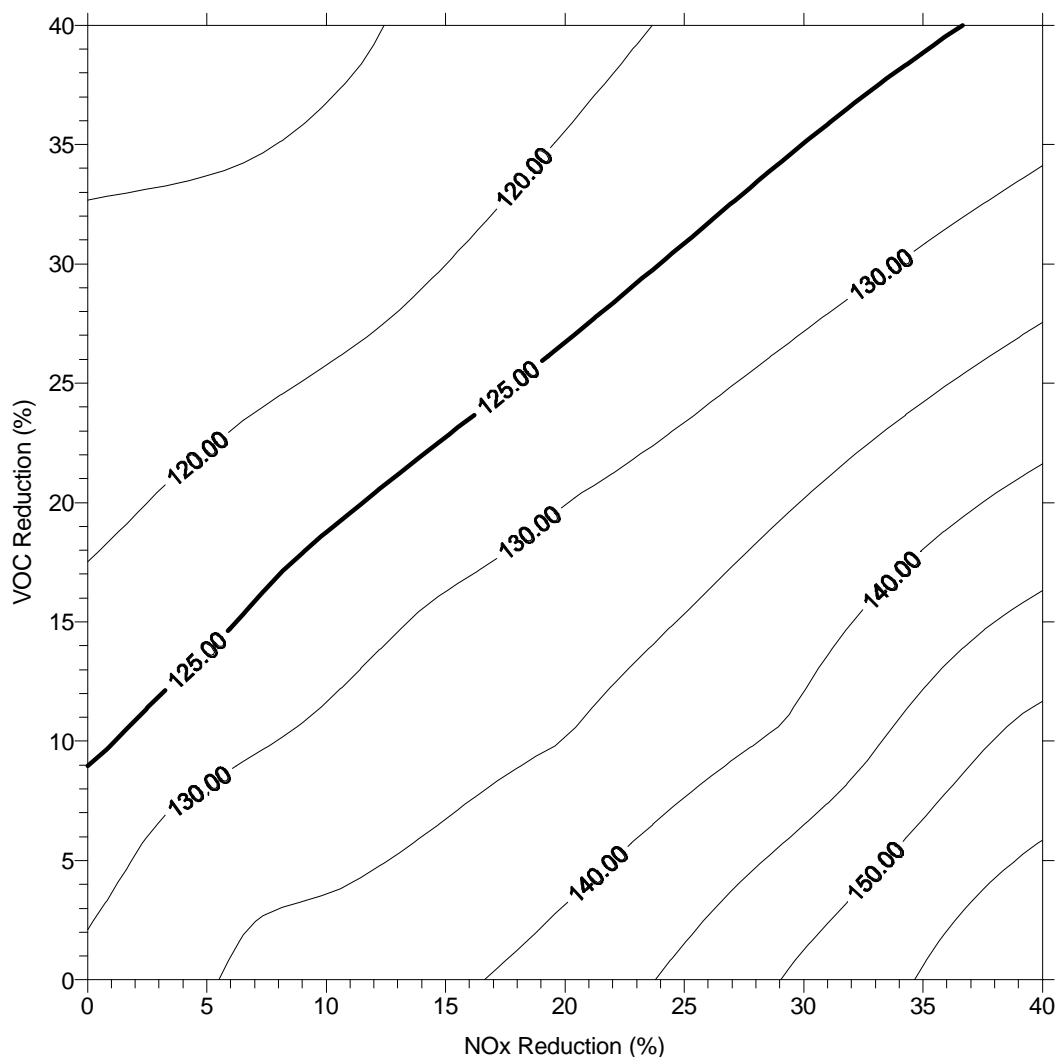
Figure 5.1. VOC vs. NOx Reductions (Episode 2, July 21 - 22, 1988)

2.   Chlorine that is emitted on the western edge of the domain does not appear to contribute to the ozone production in the urban area, with wind fields conducive to days on which ozone episodes occur. Most of the ozone increases and some decreases associated with the chlorine emissions are localized (within very few kilometers).

3.   Although the model performance evaluations are encouraging, use of the model at this time should be confined to general conclusions, such as airshed trends. In particular, the model should not be used, at the present time, to make micro-control strategy decisions. This is due to the uncertainty shown in the performance evaluation, especially in relation to its inability to reliably predict the timing of peak concentrations and location within a few grid cells.

4.   Although peak ozone values, as simulated by the model, occur somewhat later in the afternoon than the observed values, the simulated concentrations seem reasonable both in space and time.

5.   Further improvements can be made in the use of the model in the development of a new episode for 1996. Over the last year more meteorological data has been gathered for the area with the express purpose of being used in the UAM-IV.

6.   Although the emissions inventory development for the model represents the state of the science, further improvement can probably be made by incorporating studies and sensitivity analyses done recently in other areas such as Phoenix, Arizona.

The UDAQ staff is cautiously optimistic about the current results. With the recent improvements in the monitoring networks, ambient and meteorological, combined with the invaluable lessons learned by applying this very complex model to an even more complex domain, associated improvements in model performance and utility are anticipated with future efforts.

6. RECOMMENDATIONS

With a base case established (July 21 - 22, 1988, reported herein), UDAQ now intends to make UAM-IV runs for 1994, 2007, 2017, and 2020 to compare with the emissions inventory approach used in the state implementation plan included with the redesignation request.

Additional tasks for the future include recommendations from the contractors. The contractors, in their final report, have made a number of recommendations, which are summarized below with UDAQ recommendations. UDAQ intends to prioritize, and implement these within its budgetary, personnel and resource constraints:

- investigate possible under-estimations of vehicle-miles-traveled (VMT)
- analyze the 1996 summer field study
- develop new episode, based upon the 1996 field study
- apply more advanced meteorological and photochemical models (e.g. MM5)
- adopt multiple analysis approaches
- develop alternative base cases for modeling studies
- review similar UAM-IV efforts in other areas
- investigate other data support (e.g. additional upper air data)
- improve upon data generated by UAM-IV preprocessors (e.g. wind and temperature fields)

REFERENCES

Guidance on Urban Airshed Model (UAM), Reporting Requirements for Attainment Demonstration, EPA-454-R-93-056, March 1994

Guideline for Regulatory Application of the Urban Airshed Model, EPA-450/4-91-013, July 1991.

Tesche, T.W., P Georgopoulos, F.L. Lurmann, and P.M. Roth, 1990. <u>Improvement of Procedures for Evaluating Photochemical Models, Draft Final Report.</u> California Air Resources Board, Sacramento, CA.

Tesche, T. W., McNally, D. E., Chinkin, L. R., Reynolds, S. D., <u>Wasatch Front Ozone Study Ozone Modeling Protocol</u>. Utah Division of Air Quality, Salt Lake City, Utah.

Reynolds, S., H.Michaels, D. McNally, T.W. Tesche, L. Chinkin, C. Jones, M. Korc, H. Main, P. Roberts, and T. Dye; Final Report, Wasatch Front Ozone Study, Volume 1. Photochemical Modeling Results; Report to the Utah Division of Air Quality, September, 1997

This page left blank intentionally

APPENDIX A

EXECUTIVE SUMMARY

Pursuant to the Clean Air Act requirements, the State of Utah is required to develop plans for attaining and maintaining the ambient air quality standard for ozone in the Salt Lake/Davis County area. The goal of the Wasatch Front Ozone Study is to implement a photochemical modeling capability that can be used to develop an improved understanding of the processes that lead to the formation of high ozone concentrations along the Wasatch Front during episodic events. In addition, this modeling capability may be used as one means for assessing the potential effectiveness of proposed emission control plans.

Analyses of available air quality and meteorological data collected during historical ozone episodes indicated that ozone levels typically build up over a multi-day period culminating with one or more days when high ozone concentrations are observed. During such periods, up slope wind flows during the day are followed by downslope, drainage flows at night. Thus, ozone and aged precursors resulting from emissions from the metropolitan area during the day may be transported back to the area during the following nighttime period. During the next day, additional precursor emissions may be added to this aged air mass yielding higher ozone concentrations. The conceptual model for this ozone build up may be likened to a "sloshing" of the urban air mass back and forth over the city.

The Urban Airshed Model (UAM-IV) was selected for use in this study. This is the U.S. Environmental Protection Agency's (EPA) guideline model for conducting urban ozone assessments. Two approaches were employed to represent the complicated wind flow fields in the region. Initially, the Colorado State University Mesoscale Model with four dimensional data assimilation (CSUMM-FDDA) was used to develop wind and temperature inputs for the UAM-IV. Diagnostic analyses indicated that the CSUMM-FDDA wind fields were not representing all the features noted in the wind observations. As an alternative approach, wind field inputs were also developed using the Diagnostic Wind Model (DWM), which is part of the UAM-IV software package. Mixing heights were estimated using the Atmospheric Boundary Layer Model (ABLM). Emissions inputs were developed using available information for mobile, stationary, and biogenic sources provided by the UDAQ and other agencies in the study area.

Three ozone episodes were selected for modeling from the historical period 1988 through 1992. Considerations in episode selection focused on data availability to support model input preparation and performance evaluation as well as the occurrence of relatively high reported ozone concentrations. The modeling periods were 23-24 June 1988, 21-22 July 1988, and 6-8 July 1989. The peak observed ozone concentrations during these three periods were 164, 143, 191 ppb, respectively.

Model performance was assessed through comparison of measured and calculated ozone, NOx, and NO2 concentrations. In applications to the three episodes using winds derived from the CSUMM-FDDA model, the UAM tended to underestimate ozone levels at the air monitoring locations. The highest concentrations calculated anywhere in the domain were only 50 to 70 percent of the peak measured values. Considering all pairs of measured and calculated ozone values exceeding a threshold of 60 ppb, the model underestimated the observed values by 15 to 25 percent. The average absolute (unsigned) discrepancies were in the range of 19 to 29 percent. Model performance for NOx and NO2 was somewhat poorer than that for ozone. EPA guidance concerning acceptable model performance suggests that the peak measured and estimated ozone concentrations in the domain should be within 15-20 percent; the model results fall outside this range. EPA guidance also suggests that the bias in ozone results should be within 5-15 percent, and the absolute error should be less than about 30-35 percent. The results using the CSUMM-FDDA winds fall outside the bias range and are within the bounds for the absolute error.

Air trajectory analyses were carried out to help diagnose the possible cause of the underestimation bias in the ozone results. The findings indicated that the air masses arriving at stations reporting high ozone concentrations had only made a single pass over the urban source area prior to arrival at the stations. This

was not in agreement with the conceptual model of air "sloshing" back and forth over the source area prior to the observation of high ozone concentrations.

To help understand how sensitive the UAM-IV ozone estimates were to the specification of the wind field inputs, a second set of wind fields were developed using the Diagnostic Wind Model (DWM). The resulting UAM-IV ozone estimates yielded higher peak values and exhibited less underestimation bias.

The processes associated with ozone formation in the Wasatch Front area are complicated and cannot be fully characterized with the historical emissions, meteorological, and air quality data bases. Key shortcomings in the available data for the 1988-1989 modeling periods are the absence of meteorological and air quality data aloft and measurements of precursor concentrations for organic species. Such information is needed to better understand the three-dimensional dynamics of the atmosphere, to help specify suitable model inputs (such as boundary concentrations), and to provide a good basis for evaluating meteorological and photochemical model performance and diagnosing the possible causes of model performance problems.

At the outset of the study, there was an expectation that the enhanced representation of atmospheric dynamics provided by the CSUMM-FDDA approach would yield more reliable wind field estimates, especially in areas where there were no observations. This expectation has not been realized in the Wasatch Front area. A comparison of wind model results using the available observations suggests that the DWM winds are more frequently in better agreement with the observed values than the CSUMM winds.

Magnesium Corporation of America (MagCorp) operates a facility located about 90 km to the northwest of Salt Lake City near the western shoreline of the Great Salt Lake. To assess the potential importance of this source on ozone formation in the study domain, additional chemical reactions were incorporated into the Carbon-Bond mechanism to simulate the effects of chlorine chemistry. Since the chemical reaction mechanism cannot be easily modified in the nominal UAM-IV computer codes, the Flexible Chemical Mechanism (FCM) version of the UAM-IV (FCM/UAM-IV) was used in this investigation. Simulations with FCM/UAM-IV were conducted for the 21-22 July 1988 ozone episode period, both with and without the chlorine and hydrochloric acid emissions from MagCorp. When the chorine and hydrochloric acid emissions from MagCorp were included in the UAM simulation, calculated ozone concentrations in the vicinity of the facility were generally lower than those produced by the simulation with no emissions from MagCorp. This resulted from chemical reactions of Cl (a product of Cl_2 photolysis) with ozone in the plume immediately downwind of the plant. There was also a small area of higher ozone concentrations (as much as 13 ppb) near the facility.

Enhanced production of ozone by chlorine chemistry is most likely to occur in a situation where the chlorine is mixed in an air mass with significant amounts of ozone precursors. Based on wind fields generated using the DWM for the 21-22 July 1988 period, the plume from MagCorp was situated in the western portion of the modeling domain and did not mix with air containing ozone precursors emitted from sources in the metropolitan Salt Lake City area.

Recommendations for future work based on the findings of this study include:

3   Investigate the possible underestimation of vehicle miles traveled, as evidenced from the calculations performed using fuel sales and fleet fuel economy information.

4   Analyze the data collected during the summer 1996 field study sponsored by the UDAQ.

5   Apply the UAM-IV model to one or more of the periods when field measurements were conducted during the summer of 1996 and evaluate model performance. Assess the adequacy of model performance and the need for an expanded field measurement program in the Wasatch Front area to support future modeling activities.

6   Apply more advanced meteorological and photochemical models to the study area. Note that a more comprehensive set of meteorological and air quality data than that currently available will be

needed to fully realize the benefits offered by such approaches.

7   Adopt multiple analysis approaches in ozone planning activities. Examine data-based approaches that rely solely on ambient air quality data to provide information concerning the relative effectiveness VOC and NOx emissions reductions. Seek corroboration of results from alternative approaches.

8   Develop alternative base cases for photochemical modeling studies. Alternative base cases for a particular episode employ "equally plausible" inputs and yield comparable model performance. Examine effects of proposed emission control plans using the alternative base cases as a means for assessing the robustness of the modeling results.

9   Move the western boundary to the west in order to contain the entire MagCorp plume within the modeling domain. Rerun the FCM/UAM-IV simulations to evaluate the impact of the plume on ozone formation. Review data collected in the summer 1996 field study to assess the impact of the plume from the MagCorp facility on ozone formation. If the data are not adequate for that purpose, consider supporting further measurement studies of the MagCorp plume. Examine historical meteorological data to determine if conditions exist when the MagCorp plume is likely to mix with the urban plume from the metropolitan Salt Lake City area. Consider applying the FCM/UAM-IV model to such conditions if an adequate data base exists to support such a study.

APPENDIX B

ACRONYMS

ABLM	**Atmospheric Boundary Layer Model**
best9	**Best of 9 interpolation procedure**
CSUMM	**Colorado State University Mesoscale Model**
CBM4	**Chemical Bond Mechanism - IV**
Cl_2	**chlorine**
DAQ	**Division of Air Quality**
DEQ	**Department of Environmental Quality**
DWM	**Diagnostic Wind Model**
EPA	**Environmental Protection Agency**
FCA	**Flexible Chemical Mechanism**
FDDA	**Four Dimensional Data Assimilation**
MagCorp	**Magnesium Corporation of America**
NAAQS	**National Ambient Air Quality Act**
NO_x	**oxides of nitrogen**
NO_2	**Nitrogen-dioxide**
O_3	**ozone**
PM_{fine}	**fine particulate matter**
ppb	**parts per billion**
SLCIA	**Salt Lake City International Airport**
UAM	**urban airshed model**
UDAQ	**Utah Division of Air Quality**
UDEQ	**Utah Department of Environmental Quality**
VMT	**vehicle-miles traveled**
VOC	**Volatile organic compound**
w4	**Weighted-4 interpolation procedure**
WFOS	**Wasatch Front Ozone Study**